1.0

1.1

1.25

2.8   2.5

3.2   2.2

3.6

4.0   2.0

1.8

1.4   1.6

MICROCOPY RESOLUTION TEST CHART

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The Compton Defect Problem has been studied in several different approximations. Within the EH approximation, we have obtained an analytic expression for the "local maximum" Compton defect at high momentum transfers. This analytic result gives good agreement with the electron scattering helium data at large angles, and reasonable agreement with the lithium and beryllium Compton defects determined from x-ray measurements. We have also performed very careful EHS defect calculations in helium by determining the center of gravity of the Compton profile in the same manner as the experiment. (over)
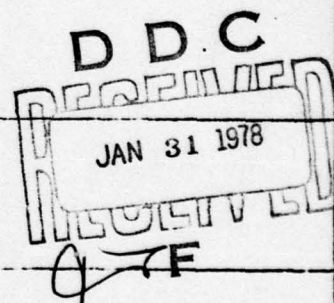
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Abstract(continued)

Our theoretical EHS results mirror the experimental values, running between 1/2 to 3/4 of the small experimental values over a range of momentum transfers going from about 2 to 13 a.u. We consider this to be a significant achievement. We have earlier predicted the neon Compton defect would be positive in sign and we have learned very recently that the experimentalists have observed this to be the case. We discuss two simple models utilized by others to explain the defect and point out the inconsistencies in each of them. We present the EHS high momentum transfer results for krypton in order to observe the convergance of $J(0)$ toward impulse values. We present a table of coefficients useful for making approximate corrections to impulse at high momentum transfers.

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Title: IMPROVED CALCULATIONS OF X RAY AND INELASTIC
      ELECTRON SCATTERING COMPTON PROFILES

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I. INTRODUCTION

The major part of our effort has gone into areas A (calculational improvements) and D (Compton defect studies) of last year's proposal. More accurate high order Bessel function generating routines have been incorporated into our codes. Calculations have been performed for photon energies up to 160 kev or more. A careful study of the dependence of our computational results on integration grid size has been done. EHS (Exact Hartree-Slater) computations[1] on the HEEIS (high energy electron impact spectroscopy) helium Compton profile measurements of Wellenstein and coworkers[2,3] have given remarkably good agreement with the small measured Compton defects over a wide range of momentum transfers. In addition we have obtained analytic Compton defect results in the hyrogenic approximation[4] valid for large momentum transfers which fit the higher momentum transfer helium experimental results quite well. This atomic model also gives reasonable results for the experimental x-ray defects in lithium and beryllium.[5] All the aforementioned experimental defects are negative in sign. In a recent paper[6], we predicted the neon defect would be positive in sign. Wellenstein has recently completed an electron scattering defect measurement in neon[7] and it does indeed turn out to be positive. Both R. Weiss, one of the leading x-ray experimentalists, and H. Wellenstein, one of the leading HEEIS experimentalists, told me in phone conversations in late December, that <u>they now agree</u> that my approach is the correct one for understanding the Compton defect. Formerly both groups[2,5] attempted to explain their defect data qualitatively via a simple "spectator electron" model, which views correlation as the cause of the defect. We shall point out some inconsistencies in this model later in this report. In addition the "spectator electron" model does not give the correct sign of the neon defect. A kinematic model developed in the 1930's[8,9] has been cited by some authors[10] to show that the Compton defect

due to binding effects must be equal to the binding energy. We shall also discuss this model and point out the inconsistency in it. In the last section, we discuss EHS corrections to impulse and provide a table of coefficients for the leading correction term for orbitals of the L and M-shells.

II. THE COMPTON DEFECT PROBLEM

The term Compton defect itself is a source of some confusion. Originally thought of as the shift in the profile maximum from that given by the scattering from a free electron at rest ($q=0.0$), the experimentalists usually measure the defect by calculating the displaced center of gravity of the profile from their experimental data by integrating over a considerable part of the profile from $-q_o$ to $+q_o$.

A paper of ours[6] came out in August 1977,

> L.B. Mendelsohn and H. Grossman, The Compton
> Defect in Aluminum, in MOMENTUM WAVE FUNCTIONS
> (AIP Conf. Proc. 36, edited by D.W. Devins),
> 249-55 (1977).

which discusses some of the early history of the defect measurements. We reported our EHS aluminum defect calculation results. The sign of the defect was correct but it was difficult to draw any conclusions on our accuracy because of the large error bars associated with the experimental result, and because we obtained a local maximum result from an extremely flat profile. The experimental defect result was based on a center of gravity computation. We also reported on the systematics of our EHS Compton defect calculations which showed that individual s orbitals lead to negative defects whereas p orbitals give rise to positive defects. We noted that for the rare gases such as neon and argon, the positive shift due to the 6 p electrons in the outer shell outweighs the negative

shift due to the 2 outer s electrons - leading to a positive defect. We include a reprint of this paper as Progress Report 77-2. At the time that preliminary results were first presented at the Seminar on Momentum Wavefunctions, held at the University of Indiana in June 1976, they were viewed with some skepticism by the x-ray and electron scattering experimentalists, who up until that time had observed only negative shifts in materials such as aluminum, lithium, and beryllium. In He and H_2, only negative defects had been observed at all but the lowest value of momentum transfer, where the defect becomes positive but quite small.

Negative Compton defects in lithium were observed independently by Weiss and Cooper, each using MoK_β x-ray radiation. Weiss observed a defect of -10 ± 3 ev and Cooper a defect of -12.4 ± 2 ev. In their paper[5] published in September 1977, they point out that it would take an underestimate of 2° in the measurement of the scattering angle to account for an observed 10 ev defect. In addition similar defects were found by both investigators in polyethylene. Weiss also observed a -10 ± 3 ev defect in beryllium when MoK_α radiation was used. They suggested a possible explanation of the effect may be due to the recoil momentum transferred from the outgoing electron to the other electrons (spectator electrons) in the atom or solid and may therefore be viewed as a many-body correction to the impulse approximation.

The high energy electron impact spectroscopy (HEEIS) Compton profile determinations of Bonham and coworkers[11,12], have been extended within the last 3 years by Barlas, Rueckner and Wellenstein[2,3] at Brandeis. Utilizing a 35 kev electron beam and constructing an apparatus which has an angular measurement precision of $.001^o$ and an energy analyser accuracy of 1ev (at a scattering angle of 12°), these very recent HEEIS Compton profile measurements are most accurate, especially for gaseous targets. For

Scattering from helium, at momentum transfers of 8.9 a.u. (10°), 10.7 a.u. (12°) and 12.4 a.u. (14°), negative defects of $-5.1 \pm$ 1ev, $-5.5 \pm$ 1ev and $-6.0 \pm$ 1ev are found. The defect remains negative and decreases with smaller angles until in the region of momentum transfer less than 3 a.u. the defect appears to change sign. For H_2, they again find negative values for the varying from -1.9 e.v. at $\theta=2.5^{\circ}$ to -4.6 e.v. at $\theta=14^{\circ}$. Again at small scattering angles, for $\theta=1.5^{\circ}$, the defect changes sign. For momentum transfer values larger than 3 a.u., they find that Weiss' "spectator electron" model result for the relative defect (the defect divided by the Compton shift) is in "fair qualitative agreement with the experimental result." Also since the relative defect in this model is proportional to $<1/r_{12}>$ where r_{12} is the distance between the two atomic or molecular electrons, it is expected that the relative defect in He should be twice as large as that for H_2. They observe that this is not substantiated by their experiments, but cannot be ruled out because of the large standard deviations of their H_2 data.

In addition McCarthy et al.[13] have observed positive 5 to 10 ev shifts (defects) of the quasi-free peak in the (e,2e) reaction for the scattering of 200–800 ev electrons from He, Ar and Xe. McCarthy and Bonham[10] using a distorted wave analysis have offered a qualitative explanation of these peak shifts.

Some of the above investigators have briefly discussed the effects of electron binding in connection with the Compton defect but conclude that binding effects are too small to explain the experimental defect results. Their arguments are based on the assertion that 1s and 2s shifts due to binding are of the order of 20% of the binding energy. We have recently calculated the 1s and 2s defects analytically within the "Exact Hydrogenic" approximation[14,15,16,17] and have found the defect results in atomic units,

$$\Delta E^{1s}_{defect} = -\frac{1}{6} \left\{ Z^{*\,2}_{1s}(0) \right\} \tag{1a}$$

and

$$\Delta E^{2s}_{defect} = -\frac{9}{10} \left\{ \frac{1}{4} Z^{*\,2}_{2s}(0) \right\} \tag{1b}$$

where the terms in the brackets represent the effective binding energies. Since these terms are greater than the true binding energies, we observe that a negative 2s Compton defect <u>greater than</u> the 2s binding energy may occur. A general analytic result[4] for K-shell and L-shell electrons has been obtained which indicates that 2p electrons exhibit positive Compton defects. These results have been obtained for the case that the (momentum transfer)^2 is much greater than the binding energy.

Table I gives a comparison of our analytic Exact Hydrogenic results, obtained in the limit of high momentum transfers, with the experimental results. The only direct comparison of these Exact Hydrogenic results with an experiment performed on an atomic gas, helium, shows them to be quite accurate at high momentum transfers. For the solids lithium and berylium, our Exact Hydrogenic atomic model appears to give reasonable results for the Compton defect, our results for beryllium falling within the stated experimental error bars. We find these comparisons to be quite encouraging.

III. EXACT HARTREE-SLATER (EHS) CALCULATIONS OF THE COMPTON DEFECT FOR HELIUM

H. Wellenstein and coworkers[2,3] have recently obtained the experimental Compton defect for helium at various scattering angles (momentum transfers) by determining the center of gravity of the top 80% of the profile, at all but the smallest values ($\varkappa < 3.0$ a.u.) of momentum transfer. We have performed

first Born calculations (EHS method) using Hartree-Slater ground state and continuum wave functions, the latter generated as a sum of many partial waves, to obtain the Compton profile $J(q)$ over the region $q=-2.5$ to $q=+2.5$. We have then obtained the center of gravity of the profile from the usual expression

$$\Delta q = \frac{\int_{-q_0}^{+q_0} q \, J(q) \, dq}{\int_{-q_0}^{q_0} J(q) \, dq} \tag{2}$$

where q_0 is chosen so that $J(q_0)$ equals approximately 20% of $J(max)$, the maximum value of the profile.

For the helium problem (2 K-shell electrons), we can apply a simple procedure to test the numerical accuracy of our EHS partial wave calculations. We can apply the partial wave procedures to the simpler hydrogenic problem, where an exact analytic expression[14,18] is known. We refer to the former calculation as Partial Wave Hydrogenic (PWH) and the latter as Analytic Hydrogenic (AH). The comparison of the AH and PWH profiles for three values of the momentum transfer is given in Table II. Following Eq. (1) of reference 17, the effective charge $Z*$ for the helium problem, is taken to be $Z*(0) = 1.59$. Agreement of the PWH with AH $J(q)$ results appears to be good to about 1 in the third figure over the whole profile. At many points, the agreement is much better than this. This excellent agreement comes from our choice of integration grid mesh of 4/1000 of a Bohr radius out to the cutoff radius value of 10.6 Bohr radii. We found using other grid mesh values that our PWH $J(q)$ values were slightly less accurate, especially for negative values of q. Thus in our EHS calculations we used the optimum grid size determined in the hydrogenic calculations.

In Table III we give our EHS $J(q)$ results for λ=3.5670 where the obvious asymmetry, with $J(-q)$ lying above $J(+q)$ at all points on the profile up to $|q|$=1.4, is clearly shown. Table IV gives our EHS defect results and compares them with the experimental results. Clearly the EHS defects mirror the experimental ones, running from about 1/2 to 3/4 of the experimental values. At the lowest value of the momentum transfer, the experimental defect surprisingly becomes positive but very small, with the value Δq=0.0 included within the experimental error bars. Our EHS defect results at λ=2.2575 gives 0 to three figures after the decimal point. A closer look at the profile itself shows that the very small asymmetry has changed to the plus side, that is with $J(+q)$ greater than $J(-q)$.

We believe that the above results demonstrate that the EHS method explains the experimental defect results in helium. We note that AH defect results have also been obtained by integrating over the top 80% of the AH $J(q)$ profile. Our AH results are typically more negative than the EHS results for the defect and are in slightly poorer agreement with experiment at the smaller values of momentum transfer.

In Table V we compare AH and PWH $J(0)$ results over a range of momentum transfers running from 2.6575 a.u. to 60 a.u. We note that with our new Bessel function generating routines, our partial wave results for this very spread out ground state wave function are quite reliable, even at the largest momentum transfer values. A less optimum choice of grid gives $J(0)$ results at the highest momentum transfers of 1.062. Note that AH $J(0)$ results are converging to the Impulse hydrogenic $J(0)$ value of 1.068 (with $Z^*(0) = 1.59$) as per the theorem we've proved earlier[14]. The number of partial waves required for PWH convergance to 4 figures is also given in Table V and is approximately proportional to momentum transfer, equal in this case to about $4 \times \lambda$.

IV. A DISCUSSION OF THE "SPECTATOR ELECTRON MODEL" AND "KINEMATIC MODEL" EXPLANATIONS OF THE DEFECT

R.J. Weiss[5] Has introduced the "spectator electron" model to explain the Compton defect. The basic idea of the model is that during the collision, the struck free elctron 1 (with momentum $\vec{P_1}$ after the collision) shares its momentum with one nearby average spectator electron 2, transferring to it momentum $\vec{P_2}$ via the Coulomb interaction. Clearly this mechanism attributes the defect to correlation.

Taking $\vec{k_0}, E_0$ as the momentum and energy of the incident photon and $\vec{k}, E$ as the momentum and energy of the scattered photon, we can write the momentum conservation equation as

$$\vec{k_0} = \vec{k} + \vec{P_1} + \vec{P_2} .$$ (3)

Here we have taken the momentum of electron 1 prior to the collision as zero. Squaring Eq(3) and noting that P_2, the momentum imparted to the spectator electron is much less than P_1,

$$(\vec{k} - \vec{k_0})^2 \sim P_1^2 + 2\vec{P_1} \cdot \vec{P_2} .$$ (4)

Now the energy conservation equation reads

$$E_0 = E + P_1^2/2 + P_2^2/2 .$$ (5)

Again dropping the P_2^2 term and substituting for P_1^2 from Eq.(4) we obtain

$$E_0 - E \doteq \frac{(\vec{k} - \vec{k_0})^2}{2} \left[1 - \frac{2\vec{P_1} \cdot \vec{P_2}}{(\vec{k} - \vec{k_0})^2} \right] .$$ (6)

Since the leading term on the right side of the equation represents the non-relativistic Compton shift for a free electron at rest, it is the second term in the parenthes which gives the defect. The remainder of the derivation uses the concepts of collision time and collision distance to evaluate the momentum P_2 transferred to the spectator electron. The energy gained by the spectator electron is taken as the Coulomb Force x

collision distance. We won't repeat the details here but clearly some
expectation value of r_{12} will enter the result. The real question is how
does one evaluate the average value of the cosine of the angle between $\vec{P_1}$
and $\vec{P_2}$. Reference 5 states that one should take the average value of the
cosine as 1/2. This implies that spectator electron 2 picks up momentum
$\vec{P_2}$ in the same general direction as $\vec{P_1}$. There is absolutely no justification
for this step. Choosing the average value as +1/2 leads to the photon
coming out with more energy than expected and therefore a negative Compton
defect in qualitative agreement with the experimental results given in
reference 5. Since there is no angular correlation between electron 1
and electron 2, the average value of the cosine should be taken as 0.
Allowing the cosine to take on all values in Eq(6) we observe that
correlation acts as a further broadening mechanism, in agreement with one's
intuition. Viewed as a mechanism to explain the defect, the effect of
correlation, via the "spectator electron model", makes no sense at all.

We shall refer to the classical model introduced by DuMond[8] and Mann[9]
to derive a Compton Defect from binding as the "kinematic model". Again
using the subscript zero to denote the quantity before the collision, the
above authors take the momentum and energy conservation equations as
follows,

$$\vec{P} = \vec{k_o} - \vec{k} + \vec{P_o} \tag{7}$$

$$E_o + P_o^2/2 - |V| = E + P^2/2 \ , \tag{8}$$

where the effect of the potential is not considered in the conservation
of momentum equation. In a straightforward fashion one finds a Compton
energy defect equal to $|V|$. $|V|$ is then taken to be the binding energy
so the shift is equal to the binding energy. In this case the photon
loses more energy than expected. Therefore the shift is to +q. The

results of this model have recently been cited to demonstrate that binding effects can't explain the Compton defect. Clearly the model is nonsense. Eq(7) is describing a free particle $\vec{P_o}$ whereas Eq(8) is describing a bound particle with momentum $\vec{P_o}$. Clearly one should also not choose $|V|$ as the binding energy since that already contains a kinetic energy contribution. The correct form of the energy conservation equation is

$$E_o - |V| = E + P^2/2 \tag{8}$$

where V is understood to be the binding energy. Now one can no longer make the substitution for $P^2 - P_o^2$ from the momentum conservation equation into the energy conservation equation to obtain the result that the defect is equal to the binding energy.

V. EHS CORRECTIONS TO IMPULSE COMPTON PROFILES

We have applied our EHS Method to the individual orbitals of krypton to study the behavior of the EHS J(0) values as we approach the impulse limit(IHS) J(0) results at high incident photon energies. Within the Exact Hydrogenic (EH) approximation, we have earlier[14,16] obtained the leading corrections analytically to the impulse hydrogenic (IH) results in the 1s and 2s cases. For the 1s case we have the result

$$\frac{J_{IH}(0)}{J_{EH}(0)} \sim 1 + .145 \left(B.E./\varkappa^2 \right). \tag{9}$$

For the 2s case, we obtained

$$\frac{J_{IH}(0)}{J_{EH}(0)} \sim 1 + .704 \left(B.E./\varkappa^2 \right) \tag{10}$$

where B.E. is the binding energy of the state and $\varkappa$ is the momentum transfer,

both expressed in atomic units. Although we have not proved this to be the case, we expect that EH corrections for all states are of the same form as those given in Eqs(9) and (10) for the 1s and 2s states.

Eisenberger and Platzmann in their work on the 1s state[18] have stated that corrections to impulse are of order $(B.E./\mu^2)^2$. However their correction refers to certain moments of the profile rather than to the profile itself.

The object of our study is three fold. Since we have obtained the limiting IHS J(0) results for the individual krypton orbitals, the comparison of EHS in the high momentum transfer region, where of the order of 100 partial waves or more must be included to achieve convergance, with IHS, serves as a check on the consistency and numerical accuracy of the EHS calculations. Second, we want to point out to experimentalists, that even at photon energies of 60 kev, corrections to impulse for the individual outermost orbitals of any atom of 1 or 2% are required. For the core the corrections for individual orbitals are significantly more. These corrections to impulse arise from including binding and using a more realistic continuum wave function to describe the outgoing electron (the EHS method). Within each closed shell, the corrections to the individual orbitals go in different directions, so that impulse remains a much better approximation for the closed shell than for the individual orbitals that comprise it. Clearly one can make a considerable error when, as is often done in Compton profile experiments in solids, one makes an impulse core subtraction for an open shell core. Finally by analyzing the convergance of our EHS results at high momentum transfers, we obtain constants C*, appropriate to the Hartree-Slater approximation, which enter the impulse correction equation with the expected form

$$\frac{J_{IHS}(0)}{J_{EHS}(0)} \sim 1 + C^*(B.E./\mu^2). \qquad (11)$$

Clearly such values of C* are very approximate, rather than exact as given by Eq.'s (9), (10) since they are obtained by fitting the data in Table VI to Eq.(11), taking into consideration the small systematic errors which appear in the numerical data. One obtains a separate C* for each state.

In Table VI, we give the EHS J(0) results for the individual orbitals (and shells) of krypton as a function of increasing incident photon energy E in kev. The scattering angle is 170°. Directly under the E's, we list the values of the associated momentum transfers $\varkappa^2$. To the right of each state we give the Hartree- Slater binding energy B.E. in atomic units. Included in the 60 kev results and to the right of the J(0) values are the precentage differences with the IHS values. The corrections to IHS for the individual orbitals of the K-shell, L-shell and M-shell are of order 15%, 7%, 2% respectively at this energy. However when one considers the individual shell contributions, the compensating effect of IHS s state profile values J(0) lying too high and IHS p state profile values J(0) lying too low are such, that the corrections for the K-shell, L-shell and M-shell are considerably reduced and are of order 5%, 2% and .7% respectively. For the closed shell atom itself, the EHS result for the L + M + N shell appears to have converged to the impulse value of 6.94. At the lower MoK$_\alpha$ energy, where only the M and N shells are excited, the IHS J(0) value falls 4% below the EHS J(0) results for the M+N shell.

Clearly for any given orbital, J(0) for large momentum transfers is converging. However a careful look at the series indicates that the apparent series limit falls slightly short of the IHS results. This can be explained by the fact that our profile numerics can be off by .002 or .003 per orbital depending on our choice of grid. For the helium problem calculation done with the PWH method where the Impulse hydrogenic result for the J(0) is 1.068, the choice of a reasonable, but not optimum, grid

gives a J(0) result at λ= 60 of 1.063. As observed in Table V, the analytic hydrogenic result at λ= 60 is 1.068. Thus our numerical procedures in PWH are giving results which are in error by about .0025 per orbital, consistent with our earlier statement. Using our high energy results, we have obtained approximate values of C* for the orbitals of the L and M shells. These are given in Table VII. Note that the C* for the 2s state in the Hartree-Slater approximation falls close to the hydrogenic value of .704. Note also that C* for a given ℓ increases significantly with increasing n. This can already be observed in the hydrogenic approximation in Eq.'s (9) and (10). We also observe that in a given shell, C* increases with increasing ℓ. Eq.(11), using the constants given in Table VII, should prove useful for making rough estimates of corrections to impulse values of J(0).

Table I. Comparison of Exact Hydrogenic Compton Defects with Experiment

Compton Defects

Atom		Experiment	Exact Hydrogenic [a]
He	$\theta=10^o$	-5.1 ± 1ev[d]	
	$=12^o$	-5.5 ± 1ev[d]	-5.7ev
	$=14^o$	-6.0 ± 1ev[d]	
Li		$-10.\ \pm3$ev[b]	
		-12.4 ± 2ev[c]	-6.1ev
Be		$-10\ \pm3$ev[b]	-12.5ev

a. Using the high momentum transfer atomic results 1a, 1b (ref 4)

b. Experiments of Weiss, ref 5

c. Experiment of Cooper, ref 5

d. Experiments of Barlas, Rueckner and Wellenstein, ref 3

Table II. Comparison of AH and PWH
Profiles for Helium (Z*(0)=1.59).

q	$\mathcal{H}$=2.6589		$\mathcal{H}$=5.3643		$\mathcal{H}$=12.441	
	AH	PWH	AH	PWH	AH	PWH
-2.5	.0000	.0000	.0000	.0000	.0246	.0245
-2.0	.0000	.0000	.0654	.0653	.0618	.0617
-1.4	.0000	.0000	.2049	.2046	.1948	.1945
-1.0	.0000	.0000	.4192	.4189	.4028	.4022
-0.7	.6727	.6718	.6588	.6580	.6412	.6405
-0.5	.8314	.8300	.8317	.8309	.8179	.8170
-0.4	.9007	.8995	.9100	.9090	.8999	.8987
-0.3	.9570	.9559	.9759	.9747	.9705	.9691
-0.2	.9961	.9946	1.024	1.023	1.024	1.022
-0.1	1.015	1.013	1.051	1.050	1.057	1.056
0.0	1.011	1.009	1.054	1.053	1.065	1.064
+0.1	.9857	.9841	1.033	1.032	1.049	1.048
+0.2	.9408	.9395	.9894	.9890	1.009	1.007
+0.3	.8798	.8789	.9275	.9271	.9487	.9473
+0.4	.8076	.8065	.8523	.8518	.8739	.8726
+0.5	.7288	.7276	.7689	.7683	.7898	.7886
+0.7	.5686	.5674	.5972	.5969	.6142	.6135
+1.0	.3630	.3626	.3756	.3754	.3846	.3840
+1.4	.1863	.1861	.1870	.1868	.1885	.1882
+2.0	.0682	.0682	.0647	.0646	.0630	.0629
+2.5	.0315	.0315	.0284	.0284	.0267	.0267

Table III. EHS Compton Profile Asymmetry for 34,500ev Electrons
            Scattering from Helium($\mathcal{K}$=3.5670)

EHS Results

$|q|$	$J(-q)$	$J(+q)$
0.0	1.062	1.062
0.1	1.052	1.042
0.2	1.014	0.995
0.3	0.953	0.925
0.4	0.876	0.840
0.5	0.790	0.747
0.6	0.703	0.654
0.7	0.618	0.566
0.8	0.539	0.485
0.9	0.467	0.413
1.0	0.401	0.350
1.2	0.291	0.252
1.4	0.214	0.182
1.6	0.0	0.132
1.8	0.0	0.096
2.0	0.0	0.070
2.5	0.0	0.033

Table IV. Comparison of Theoretical (EHS) and Experimental Compton Defects Δq for 34,500 ev Electrons Scattering from Helium

| mom transf (κ) | Defects | | EHS |
	Δq(Exp)[a]	Δq(EHS)[b]	$-q \rightarrow +q$ range
2.2575	+.007	.000	± .5
2.6589	−.018	−.013	±1.0
3.5670	−.028	−.025	±1.4
4.4699	−.027	−.021	±1.4
5.3643	−.028	−.019	±1.4
7.1235	−.019	−.014	±1.4
8.9513	−.020	−.011	±1.4
10.686	−.019	−.009	±1.4
12.441	−.016	−.008	±1.4

a. A.D. Barlas, W. Rueckner and H.F. Wellenstein, in MOMENTUM WAVE FUNCTIONS, AIP Conf. Proc#36, p241 (1977). Results reported give center of gravity of the top 80% of the profile (except for $\kappa<3$).

b. EHS results are center of gravity results for the top 80% of the theoretical profile, (except for $\kappa<3$). The q range used in the EHS calculations are given in the 4th column.

Table V.   Comparison of Partial Wave Hydrogenic(PWH) to Analytic
           Hydrogenic(AH) J(0) Values for Helium($Z^*=1.59$).

J(0)

mom transf($\varkappa$)	AH	PWH	No of Partial Waves [a]
2.6589	1.011	1.009	10
5.3643	1.054	1.053	22
12.441	1.065	1.064	52
20.0	1.067	1.065	84
40.0	1.067	1.065	166
60.0	1.068	1.066	230

a. This is the number of partial waves necessary for
   convergance to 4 figures.

Table VI. Comparison of Exact Hartree-Slater J(0) with Impulse Hartree-Slater J(0) for the Orbitals and Shells of Krypton; EHS Calculations done for Variable Incident Photon Energy E at Θ=170°.

state	B.E.	17.37	40	60	80	100	120	140	160	IHS J(0)
E(kev) →		17.37	40	60	80	100	120	140	160	
χ^2 →		180	397	841	1414	2099	2879	3745	4688	
				EHS J(0) Values						IHS J(0)
2s	135.5	.0724	.0724(-12)	.0803	.0821	.0833	.0842	.0848		.0877
2p	123.3	.0530	.0515(+17)	.0499	.0487	.0478	.0471	.0466		.0441
L-Shell		.463	.464(+6)	.467	.456	.453	.449	.449		.440
3s	19.73	.184	.206	.213(-6)	.217	.219	.220	.221		.226
3p	15.23	.154	.150	.146(+8)	.143	.141	.140	.139		.132
3d	7.098	.106	.0902	.0896(-9)	.0908	.0920	.0931	.0940		.0984
M-Shell		2.345	2.218	2.197(-2)	2.202	2.208	2.213	2.219	2.222	2.250
4s	1.946	.622 , .650		.659(-2)						.672
4p	.952	.528	.501	.494(+2)						.484
N-Shell		4.409	4.308	4.278(+.7)						4.250
L+M+N		6.99	6.94	6.94						6.94

Table VII. Coefficents to Use In Eq.(11) for Corrections to Impulse

state	C*
2s	+.8
2p	−1.3
3s	+2.0
3p	−3.7
3d	∼ +17.

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